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ON A PROBLEM OF REPEATED MEASUREMENT DESIGN WITH TREATMENT ADDITIVITY

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We consider an experimental design problem in which n treatments are applied successively to each experimental unit, and once applied their effects are permanent. To examine all $2^n - 1$ treatment combinations, a minimum of $\binom{n}{[\frac{n}{2}]}$ experimental units is both required and sufficient. A linear model is described and the first nontrivial case, $n = 4$, is examined in detail. It is shown that there are 24 nonisomorphic designs which reduce to 13 under the assumption of no interaction between the treatments. A serial correlation model is considered and the D, A and E, optimality criteria evaluated for $\rho = 0$, 0.5 and 0.75. Possible uses for the design automorphisms are then considered.

1. Introduction. This research was stimulated by a medical problem which was considered in the Statistical Laboratory of Michigan State University. An orthopedic surgeon was concerned with statistical evaluation of resultant laxity as caused by each of the possible combinations of ligamenteneous injuries of a knee. Since the experimental units were human cadaver joints it was decided that the number of them be as small as possible.

At each stage of the experiment $t \leq n$ he wishes to compare the effects of all $\binom{n}{t}$ treatment combinations. It is assumed that the resulting effect of t treatments applied at state t does not depend on the order in which they were applied. Clearly such an experiment requires at least $\max_k \binom{n}{k}$ experimental units for any n. Hence the minimum number of experimental units will equal $\binom{n}{\frac{n-1}{2}} = \binom{n}{\frac{n+1}{2}}$ for n odd and $\binom{n}{\frac{n}{2}}$ for n even. It can be shown using well known theorems on systems of distinct representatives that such a design can in fact be constructed for any n. The problem arises as to how many distinct ways such a construction can be carried out.

Similar situations may arise in other fields of application, such as education, agriculture and others. Suppose, for example, that students satisfied prerequisites for n future courses which are unrelated in the sense that none of them is a prerequisite for another. Nevertheless each course is beneficial for consecutive studies and makes a specific contribution to the success of the student in his further studies. At each stage of the experiment it is desirable to compare the combined effect of all possible courses taken by the students up to and including this stage and to investigate which sequence should be preferred, if any.

In many fields of applications the major problem to be solved by the experimenter could be how to formulate meaningful commensurate measures for the effects of each of the treatments under consideration. It seems that the prospects of applying such types of designs

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to operations research are from this standpoint more promising. Suppose that some machine has n components and the failure of each of them will affect the performance of the machine in some specific way which does not depend on the performance of the remaining components. Also the effect of failure of any subset of the components depends solely on the structure of the subset. The experimenter is interested in finding a scheme for the order of checking the components to insure the maximum reliability of the performance of the machine. He will make the decision after investigating the performance of $\max_k \binom{n}{k}$ machines in which all n components will be checked in accordance with a type of the design discussed here. In this area of research it seems natural to introduce also a cost function and a probability of failure for each component. Such ramifications may influence the choice among the designs described here.

2. The combinatorial properties of repeated measurement designs for $n = 4$. We have studied the case $n = 4$ principally because this is the simplest nontrivial situation. Since $\binom{4}{2} = 6$ is the maximum value of $\binom{4}{t}$, $t \leq 4$, it is clear that at least six experimental units are required.

At the first stage of the experiment the problem is that the number of experimental units is not divisible by the number of treatments. It seems therefore reasonable to assign at random two treatments each to two and two to one experimental unit. We may therefore assume without loss of generality that treatments 1 and 2 were assigned to two units, and 3 and 4 to one unit only. At the second stage of the experiment we should assign the treatments to the experimental units in such a way that the six unordered pairs occur. Now the problem is in how many distinct ways this can be carried out. To enumerate all possibilities we first assume that to one of the units we apply treatment 1 followed by treatment 2, and then see in how many ways we can proceed in order to obtain the six distinct pairs. It is easy to see that this yields twelve possibilities. By symmetry there will also be twelve possibilities in which we have a unit with treatment 2 applied at the first stage and treatment 1 at the second. Hence in total there are twenty-four possibilities for the second stage of the experiment. We shall exhibit next the first twelve possibilities. The remaining twelve are clearly obtained by interchanging the assignments of the treatments to the first and second stage of the experiment. To each of the cases shown in Table 1 there will be a corresponding one obtained from it by interchanging the first and second columns. We shall number the case corresponding to the ith possibility by i'; $i = 1, 2, \cdots, 12$. Since the order of S_4, the symmetric group of degree four, is twenty-four, it is clear that the enumeration could have been obtained by making any of the sets of six pairs correspond to the identity, and using the elements of S_4 to obtain the remaining sets. We shall use hereafter an inverse of this function. We shall choose the first set as corresponding to the identity of the permutations group of degree four, and from here on, associate with each of the remaining sets that permutation which will change that set into the first set. This will yield the results in Table 2. The problem now is how to proceed to the third and fourth stage of the experiment.

The aim is to apply to each experimental unit all four distinct treatments. Hence the two treatments applied to each unit at the first two stages determine the pair of treatments to be used in the last two stages.

Under the condition that in each column two treatments occur twice and two once, the six pairs of the last two columns will be distinct. Thus the third and the fourth column could be any of the twenty-four designs considered for the first two stages with a proper rearrangement of each set so that each experimental unit receives all four treatments.

This gives 576 designs which consist of 24 equivalence classes. Since any design of the first two stages can be transformed to design 1 by the corresponding permutation we may choose a representative of these 24 classes by fixing the design at the first two stages and letting the design at the last two stages run through all 24 distinct designs. Hereafter we choose the first

TABLE 1

Number	1	2	3	4	5	6	7	8	9	10	11	12
	12	12	12	12	12	12	12	12	12	12	12	12
	13	13	13	13	31	31	31	31	31	31	31	31
	23	23	32	32	23	23	23	23	23	23	32	32
	24	42	24	24	24	24	24	42	42	42	24	24
	34	34	34	43	34	43	43	34	34	43	43	43
	41	41	41	41	41	41	14	41	14	14	14	41

TABLE 2

Number of the set	1	2	3	4	5	6	7	8	9	10	11	12
Corresponding permutation	I	(1234)	(23)	(124)	(1432)	(142)	(34)	(13) (24)	(1243)	(234)	(123)	(1324)
	1′	2′	3′	4′	5′	6′	7′	8′	9′	10′	11′	12′
	(14) (23)	(13)	(14)	(132)	(24)	(243)	(1423)	(12) (34)	(1342)	(143)	(134)	(12)

design to be the design numbered 1 in Table 1. Hence the complete design consists of pairs $(1, j)$ where j assumes the values 1, $\cdots$, 12; 1′, $\cdots$ 12′.

We turn now to the statistical aspect of the problem. Are these 24 designs equivalent for statistical purposes although distinct structurally? Should we give the usual advice to the experimenter to choose any of these designs at random? It seems that this advice was never satisfactory because it ignored the information built into the specific design used which may have been inconsistent with the problem considered by the experimenter. We shall make this point clearer by examining the present case. It will emphasize that the choice between designs having the same structural parameters should be made in accordance with the statistical model and the statistic used as a basis for the decision.

We remark here that these 24 distinct designs could be used for problems of two-way classification with four treatments, six rows and four columns. The designs constructed here possess all but one property of GYD. The number of times two treatments occur together in columns is not constant. If one intends to use these designs for eliminating two-way heterogeneity, then usually the decision regarding no difference between treatments is based on the generalised variance statistic. This statistic is invariant under interchanging rows or columns of the design. Hence it seems natural to introduce an additional identification of the designs beyond fixing the first two columns. We may consider two designs the same if they are obtained from each other by interchanging the last two columns. This gives only 12 distinct designs. However, the generalised variance statistic is not sensitive to the different structures of the last two columns. We find that the determinant of the corresponding information matrix (computed under the standard "blocks plus treatment effects" model rather than the model we describe in Section 3) assumes just two values. For four of the designs the value of the determinant equals 192 and for eight of them 192⅔. The eigenvalues of these matrices are proportional to 16, 18, 18 and 17, 17, 18 respectively. Hence using the D, A or E optimality criteria, we would conclude that the designs of the second group are better. In fact, since $f(16) + f(18) \geq 2f(17)$ for any convex function f, the second group dominates the first with respect to a very wide class of criteria. In particular, since the information matrix is completely symmetric (c.s.) for this model, the second group is "universally optimal." See Kiefer (1975), Proposition 1.

Examining closer the structure of the two groups, we find among the first group two designs which have an additional symmetry beyond the one built into these designs by our construction. These two designs have four pairs of columns consisting of six distinct pairs of treatments. The remaining designs have just two pairs of such columns, a property imposed on these designs by construction. Since there is no other obvious property separating the remaining designs one could expect that a criterion of optimality would single out just these two designs from the others. An explanation why this additional symmetry did not have any effect on the optimality of those designs could be that one cannot expect that a model will bring out a property which was not built into it. The model for eliminating two-way heterogeneity is not sensitive to the relative structure of the columns.

In the next section we shall formulate a linear model for the type of designs considered here. The invariance of the information matrix under the assumption of no interaction between treatments will induce additional identification of the designs beyond the relabelling which reduced the number of the equivalence classes to 24. The information matrix remains the same if we interchange the first two columns with the last two columns or interchange the order within the first two columns and the last two columns. Presently we shall express this property with respect to the combinatorial structure of the designs. It is enough to express the identification of two complete designs when both are in a standard form, i.e., $(1, j)$. We shall consider two designs the same, i.e., $(1, a) = (1, b)$ in the following cases:

(i) $B^{-1} = A$

(ii) $(B')^{-1} = A[(14)\,(23)]$

(iii) $(14)\,(23) = A(B')^{-1}$

where A, B, B' denote the permutations which change two columns of the form a, b, b' into columns of form 1 in accordance with Table 2. (i) expresses the property that we may interchange the first two columns with the last two. (ii) means that we may interchange the

order within the first two and the last two columns. (iii) means that in addition to operation (i) we also perform operation (ii).

This identification reduces the 24 equivalence classes to 13 with the classification shown in Table 3, where design $(1, j)$ is denoted (j).

3. Formulation of the linear model. Let $y_i = (y_{1i}, y_{2i}, \cdots y_{ni})^T$ be the column vector of observations on the ith experimental unit, and consider the case $n = 4$, with design specification "1234" for the ith unit. Then, omitting the interaction terms, we shall suppose that the mean vector is defined by $E(y_{1i}) = \mu_i + \alpha_1$, $E(y_{2i}) = \mu_i + \alpha_1 + \alpha_2$, $E(y_{3i}) = \mu_i + \alpha_1 + \alpha_2 + \alpha_3$ and $E(y_{4i}) = \mu_i + \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4$. With obvious modification for alternative design specifications, we see that the principal property of this model is its order invariance for given mean. For example, the designs "1324," "2134," "2314," "3124" and "3214" will all give the same value for $E(y_{3i})$ as given above. Interaction terms can be introduced in an obvious manner, and hence for general n we can write our model in the form

$$\mathbf{y}_i = \mu_i \mathbf{1} + X_{1i}\boldsymbol{\alpha} + X_{2i}\boldsymbol{\beta}_2 + X_{3i}\boldsymbol{\beta}_3 + \cdots + X_{ni}\boldsymbol{\beta}_n + \mathbf{e}_i; \qquad i = 1, \cdots, m,$$

where μ_i corresponds to a "row effect" in the design layout, $\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_n)^T$ is a vector of main effects for the treatments. $\boldsymbol{\beta}_j$ *is an* $\binom{n}{j}$-vector of order invariant j-way interactions ($j = 2, \cdots, n$), $\mathbf{1}$ is an n-vector of 1's, X_{ji} is an n by $\binom{n}{j}$ design matrix of 0's and 1's as determined by the additivity assumptions and the order in which the treatments are applied ($j = 1, \cdots, n$), $\mathbf{e}_i$ is a random n-vector with zero mean and variance matrix Σ, and $m = \binom{n}{[\frac{n}{2}]}$ is the number of experimental units. This model is related to the standard "Repeated Measurement" model with residual effects.

It is clear that this model is heavily over-parameterised, even with the usual constraints on the main effects and interaction terms. One appropriate simplification for the interactions would be to assume invariance under relabelling for terms of a given order. So that we can write $\boldsymbol{\beta}_j = \beta_j \mathbf{1}$, and hence

$$\gamma_i = \mu_i \mathbf{1} + X_{1i}\boldsymbol{\alpha} + X^*_{2i}\boldsymbol{\beta} + \mathbf{e}_i; \qquad i = 1, \cdots, m,$$

where $\boldsymbol{\beta}$ is now an n-vector equivalent to a "column effect" in the design, and X^*_{2i} is an $n \times n$ matrix of 0's and 1's. Note that this model will differ from the standard model for two-way heterogeneity in that X_{1i} will be some column permutation of the matrix whose jth column ($j = 1, \cdots, n$) is $(0, \cdots, 0, 1, \cdots 1)^T$—that is $(j - 1)$ 0's followed by $(n - j + 1)$ 1's—as opposed to being some column permutation of the identity matrix.

An alternative restriction on the interaction terms in the original model would be simply to omit those of third order or higher. This alternative would place greater emphasis on balancing the design with respect to pair selection, but at the expense of increasing the dimensions of the X^*_{2i} matrices. And for this latter reason we have concentrated on the first proposal for simplification in our search for an optimal design.

We shall now assume that for the purpose of selecting an optimal design the parameter of interest is $\boldsymbol{\alpha}$. Then, assuming observations on distinct experimental units are uncorrelated, the variance matrix, V, for the usual least-squares estimator of $\boldsymbol{\alpha}$ is defined by

$$\begin{aligned}\sigma^2 V^{-1} &= \textstyle\sum_{i=1}^m (X_{1i}^T P^{-1} X_{1i}) - (\sum_{i=1}^m X_{1i}^T P^{-1} X^*_{2i})(\sum_{i=1}^m X_{2i}^T P^{-1} X^*_{2i})^-(\sum_{i=1}^m X^{*T}_{2i} P^{-1} X_{1i}) \\ &= C_d, \text{ say,}\end{aligned}$$

where $\Sigma = \sigma^{2\rho}$ and to avoid manipulations with generalised inverses we have reduced the dimensions of $\boldsymbol{\mu}$ and $\boldsymbol{\beta}$ respectively, by 1, via the side constraints $\Sigma\mu_i = \Sigma\beta_j = 0$, altering X^*_{2i} ($i = 1, \cdots, m$) correspondingly. We have assumed that Σ is known. In practice Σ could be estimated from the data, but since this paper is concerned with design selection before observing the data, we must choose some value "a priori."

TABLE 3

Equivalence class	1	2	3	4	5	6	7	8	9	10	11	12	13
Representative	(1)	(2) (5)	(2′) (5′)	(3)	(3′)	(4) (6) (10′) (11′)	(4′) (6′) (10′) (11′)	(7) (12′)	(8)	(8′)	(9) (9′)	(7′) (12)	(1′)

For appropriate restrictions on $\Sigma = \{\sigma_{rs}\}$ we turn to the closely related topic of "split-Plot" designs, and assume a "serial correlation" model, for which $\sigma_{rs} = \sigma^2\rho^{|r-s|}$ $(r, s = 1, \cdots, n)$. See, for instance, Cochran and Cox (1957) page 294. This matrix has a simple tri-diagonal form for its inverse. See Graybill (1969) page 182.

An alternative form for Σ would come from a "nearest neighbour" (NN) model, for which $\sigma_{rs} = 0$, $|r - s| > 1$ otherwise as for the "serial correlation" model. This matrix does not however have a simple form for its inverse. Kiefer and Wynn (1979) use this model but restrict attention to small ρ, which gives them a justification for using unweighted least-squares and hence no requirement for the inversion of Σ. Either model seems reasonable for our problem, and we have used the first, or "serial correlation" model, in the numerical calculations of Section 4. Note that V can be converted into a variance matrix (W say) of estimable contrasts for the α's by setting $W = BVB^T$ where B is the $(n - 1) \times n$ matrix whose jth row is (0, 0, $\cdots$, 0, 1, 0, $\cdots$, -1), with a 1 in the jth position.

4. Optimality Investigations. For numerical comparisons between different designs, the expression for C_d can be written in the form

$$a_\rho C_d = \textstyle\sum_{i=1}^m X_{1i}^T K_\rho X_{1i} - (\sum_{i=1}^m X_{1i})^T D_\rho (\sum_{i=1}^m X_{1i})$$

where a_ρ can be chosen so as to make all entries in the $n \times n$ matrices K_ρ and D_ρ, integers. In particular for $\rho = 0$ we put $a_0 = mn$ which gives $K_0 = mnI_n - mJ_n$, $D_0 = nI_n - 2J_n$ and $U_i = X_{1i}^T/k_0 X_{1i}$ has entries

$$U_{rs} = U_{sr} = (n - r + 1)(s - 1); \qquad r \geq s \qquad r, s = 1, \cdots, n$$

when the ith row in the design is $12 \cdots n$. All other U_i terms are coordinate transformations (row-column permutations) of this particular U_i.

When n is odd, n divides m and we can restrict attention to designs where all treatments occur equally often in each column of the design. We then find that

$$(\textstyle\sum_{i=1}^m X_{1i})^T D_0 (\sum_{i=1}^m X_{1i}) = -\tfrac{1}{6}m^2(n + 1)(n + 2)J_n, \qquad n \text{ odd}$$

and hence trace C_d = constant, over all such designs. For completely symmetric C_d matrices, this is a sufficient condition for all such designs to be universally optimal in the sense of Kiefer (1975), where this criterion is called Φ_{-1}^*-optimality. However, this class of designs does not appear to be (uniformly) optimal for any other Φ_p^* and hence optimal designs must be selected by direct numerical investigation with specific criteria. This is also the case for n even. Note that our designs for n odd are all regular GYD's and hence they are universally optimal for the standard "two-way heterogeneity" model. See Kiefer (1975) page 342.

Now, for $n = 4$ we have established in Section 2 that there are just 24 nonisomorphic design types. We have evaluated C_d for these 24 designs and ranked them according to their values on the following three criteria:

D-optimality: det V
A-optimality: trace V
E-optimality: maximum eigenvalue of V,

the "best" designs in each case being those with smallest scores on the chosen criterion.

For $\rho = 0$ the structure of the thirteen (reduced) equivalence classes was preserved, but with some further grouping. The rankings for each reduced class on each criterion are given in Table 4, with the rankings on A being used to order the table, as this criterion produced the finest mesh. We see that (reduced) equivalence class 8 is uniformly optimum. This result cannot be strengthened to "universal optimality" in the sense of Kiefer (1975, pages 336–338) as the ordered vector of eigenvalues for the C_d matrix of equivalence class 8 does not dominate those for the other classes.

Table 4 is little altered if W rather than V is used for the calculations. In particular, equivalence class 8 is optimum on the three given criteria but is not universally optimal.

For $\rho = 0.5$ and $\rho = 0.75$ the full set of 24 equivalence classes was required, with 20 distinct

TABLE 4

A rank	1	2	3	4	5	6	7	8	9
D rank	1	3	6 =	4	2	7	6 =	5	8
E rank	1	3	2	5 =	5 =	5 =	4	6 =	6 =
classes	8	6, 7, 11	12	2, 5	1	9	3, 4	10	13

groups emerging for $\rho = 0.5$ and 10 for $\rho = 0.75$. For $\rho = 0.5$ the prime (′) designs were uniformly better than the nonprime designs, with 8′ and 12′ (a member of the previously optimal reduced equivalence class 8) coming out first and second respectively. Since 8′ was only 0.4% more efficient than 12′ at this value of ρ whilst it was 6% less efficient than 12′ when $\rho = 0$, the design 12′ would seem a good one to select. This is confirmed by the results for $\rho = 0.75$ when (reduced) equivalence class 8 again came out to be uniformly optimum.

We now ask whether design 12′ (or equivalence class 8) has any distinguishing combinatorial properties, as this may act as a guide in selecting optimal designs for larger values of n. For this, we note the following theorem, due to Kiefer and Wynn (1979, Theorem 5.1).

THEOREM (Kiefer and Wynn). *A* BIBD *is weakly universally optimum for the* NN *model if all the quantities*

$$e_{ii'} + kN_{ii'} \qquad i \neq i'$$

are equal.

In our context, $k = n$, $e_{ii'}$ is the number of rows in the design for which i occurs at one or other end plus the number in which i' occurs at an end, whilst $N_{ii'}$ is the number of times i and i' are adjacent in a row. Of course, for $n = 4$ our designs are not BIBD nor are any of them (weakly) universally optimal. However, it is in fact easy to verify that the condition of this theorem is satisfied by all the designs in equivalence class 8.

We now turn to the case $n = 5$, for which Seiden (1979) has shown that there are 304 nonisomorphic designs, and hence searching for a design which satisfies the condition in this theorem is difficult. Further results in this case must await the results of an extensive numerical investigation.

For $n = 6$ there is every indication that the number of designs is extremely large. Furthermore, unlike the $n = 4$ and $n = 5$ cases, we cannot have either $e_{ii'}$ or $N_{ii'}$ separately all equal, making the search for a design which satisfies the condition of the theorem doubly difficult.

One can easily formulate a computer program which will enumerate all nonisomorphic designs and compare them using some optimality criteria. It is easy to show that even if one assumes $\rho = 0$, one cannot identify two designs which are obtainable from each other by interchanging two columns. We constructed six distinct designs for $n = 6$ by trial and error. All of them satisfy the basic conditions of the designs considered here, i.e., that at each stage of the design for $t < n$ each of them includes all possible t-tuples. The idea of the construction was to achieve the distribution of the $N_{ii'}$'s or $e_{ii'}$'s as symmetric as possible. It turned out, as expected, that the design with the $N_{ii'}$'s as equal as possible was uniformly best on all the criteria considered. A little distortion of it to achieve more symmetry with respect to the distribution of $e_{ii'}$'s yielded a design of much lower rank. For $n = 6$ one could still enumerate all nonisomorphic designs and find the best one. For $n > 6$ the number of designs will probably be too big to make the enumeration worthwhile. It seems therefore that for $n > 6$ one should impose more additional symmetry conditions and search for a "best" design within a narrower class in accordance with criteria relevant for the intended applications.

The somewhat anomalous results for nonzero ρ need not surprise us, as can be seen by examining the case $n = 2$ with the further simplification $\alpha_1 = \alpha_2$, so that $m = 1$ is sufficient. The BLUE for $\mu_1 + \alpha_1 (= \mu$ say) when $\rho = \frac{1}{2}$ is then just $\frac{1}{2}y_2$, which completely ignores the first observation. Such results will clearly have design implications.

We finish with a remark on the possibility of using design automorphisms to guard against experimental unit-treatment-combination interactions. The conventional approach required replication of the design, using blocks of experimental units, but suppose we can group the treatments; and that this grouping can be matched (by choice of labels) to one or more of the design automorphisms. For example, suppose (1, 2) forms one group of treatments and (2, 3) is a design automorphism, then we relabel the treatments so that the group becomes (2, 3). Since an automorphism implies that the specified treatment relabelling is equivalent to a reallocation of treatment-combinations to experimental units, we see that automorphism(s) can generate an equivalence between the homogeneities of the treatment group(s) and certain of the experimental unit-treatment-combination interactions. At the very least this should help to reduce their impact, if present, and may well leave some of them estimable without replication of the design. On this first point, we hope to show in a forthcoming paper that randomisation over the design automorphisms, in this context, will eliminate the unwanted interactions; whilst on the second point it is easy to see, for instance, that an unbiased estimate for the contrast $\gamma_{ji} - \gamma_{j'i}$ (where γ_{ji} is the interaction between the jth experimental unit and the ith treatment, and j' is the corresponding experimental unit under the automorphism) is given by $y_{ji'} - y_{ji'-1} - y_{j'i'} + y_{j'i'-1}$, where i' is the sequence number for the ith treatment on the jth experimental unit.

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